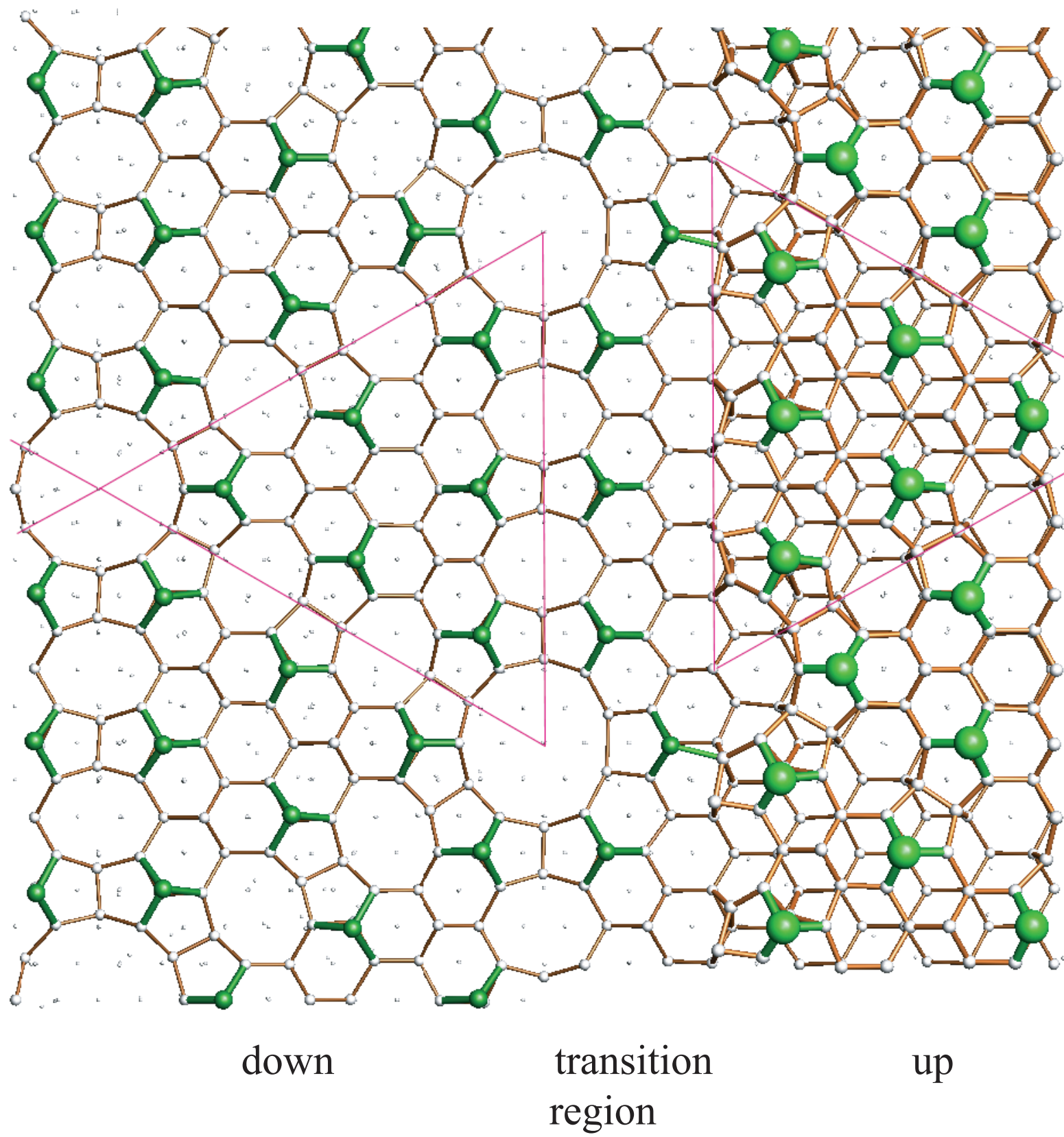


U2 || 1 step configuration for Si(111) - 7x7

Experiment

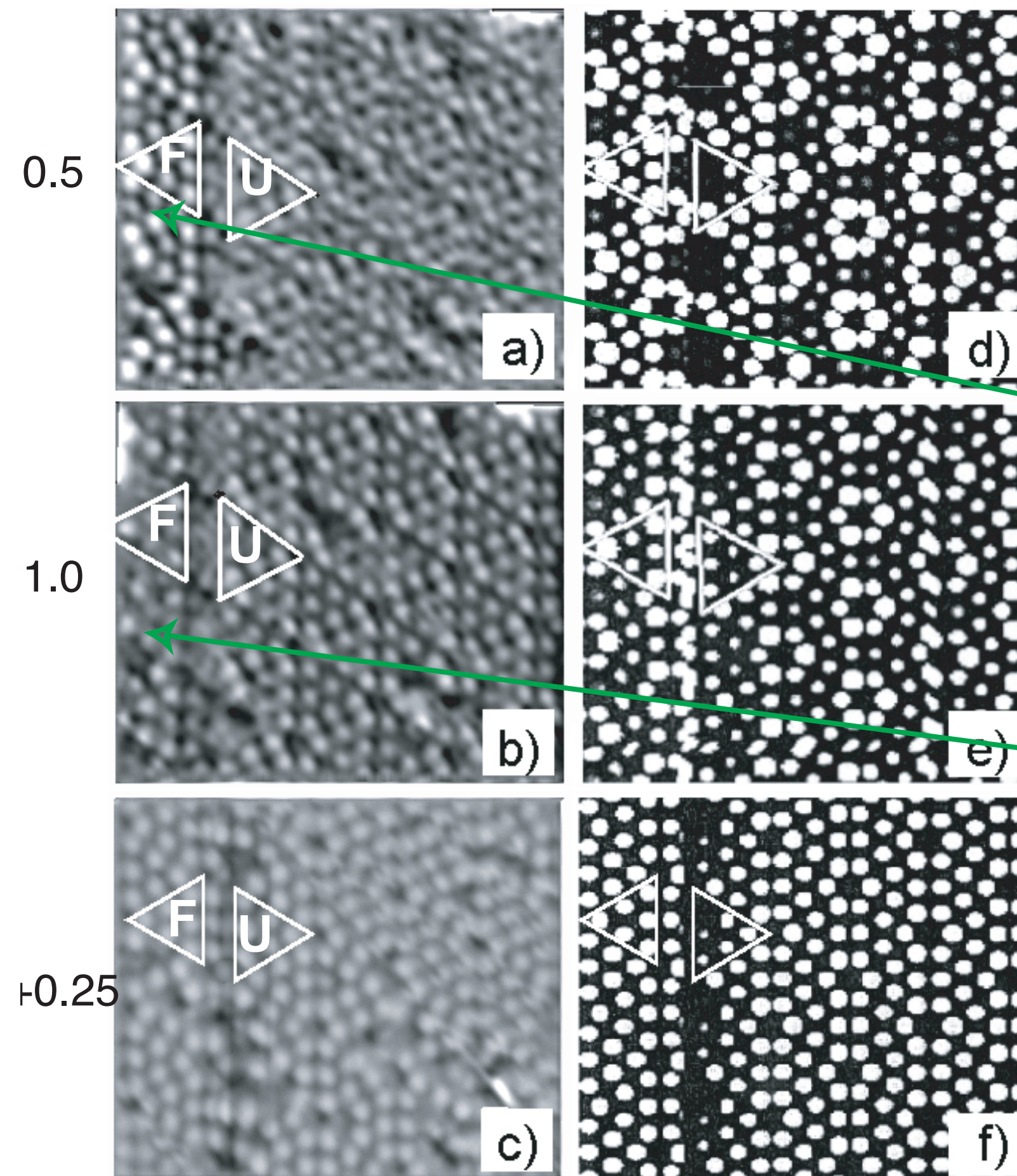
Theory

Calculated density of states



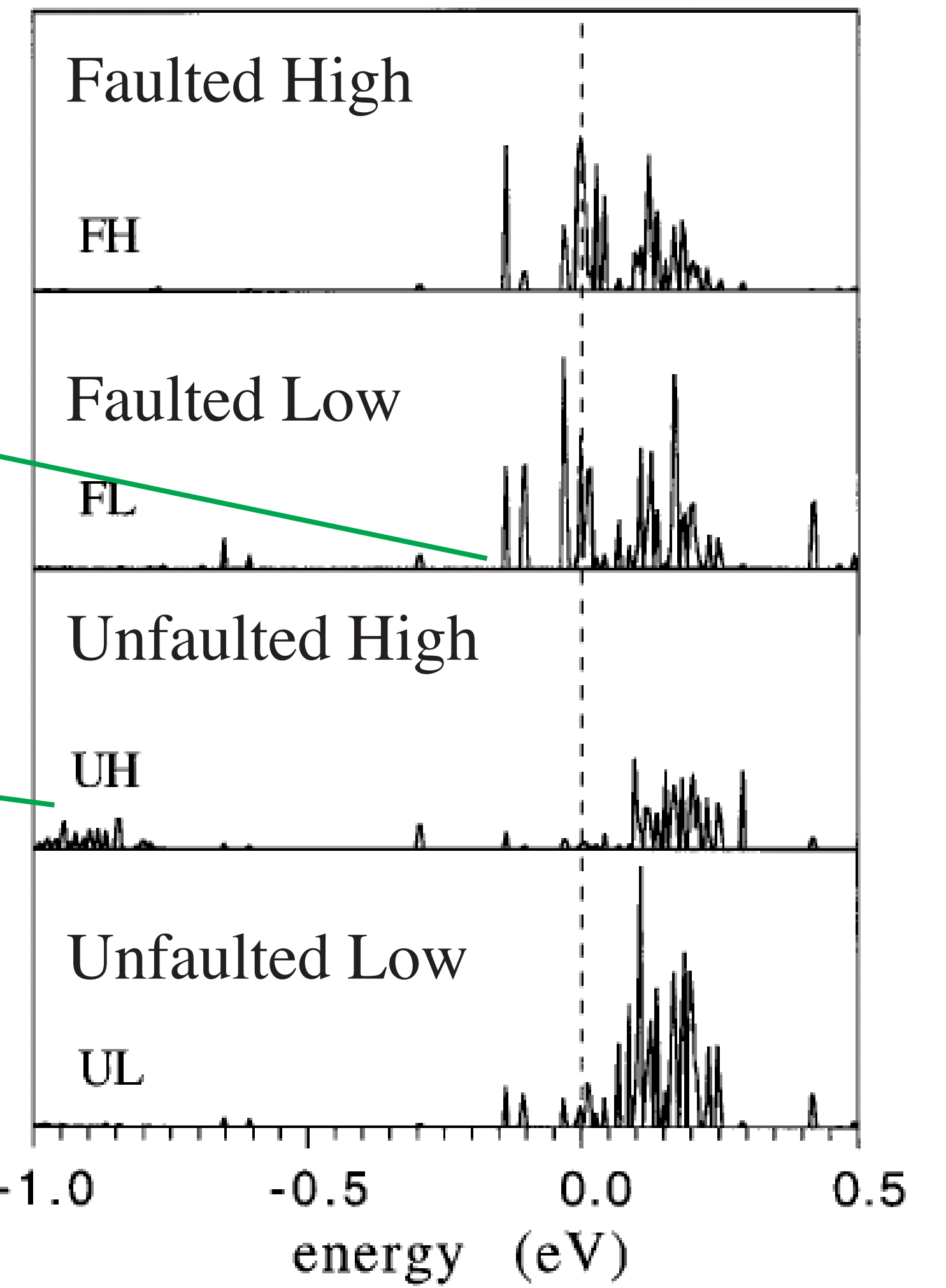
- Transition region is 2a
- Lateral shift by n=1

We have observed that the low side of the step is brighter than the high side for $V = -0.5V$ but not for $V = -1.0V$. No difference in intensity for positive voltage.



Hupalo et. al Phys. Rev. Lettr. 84, 2877 (2000)

Images of the stepped Si(111) surface as a function of the tip-surface tunneling voltage



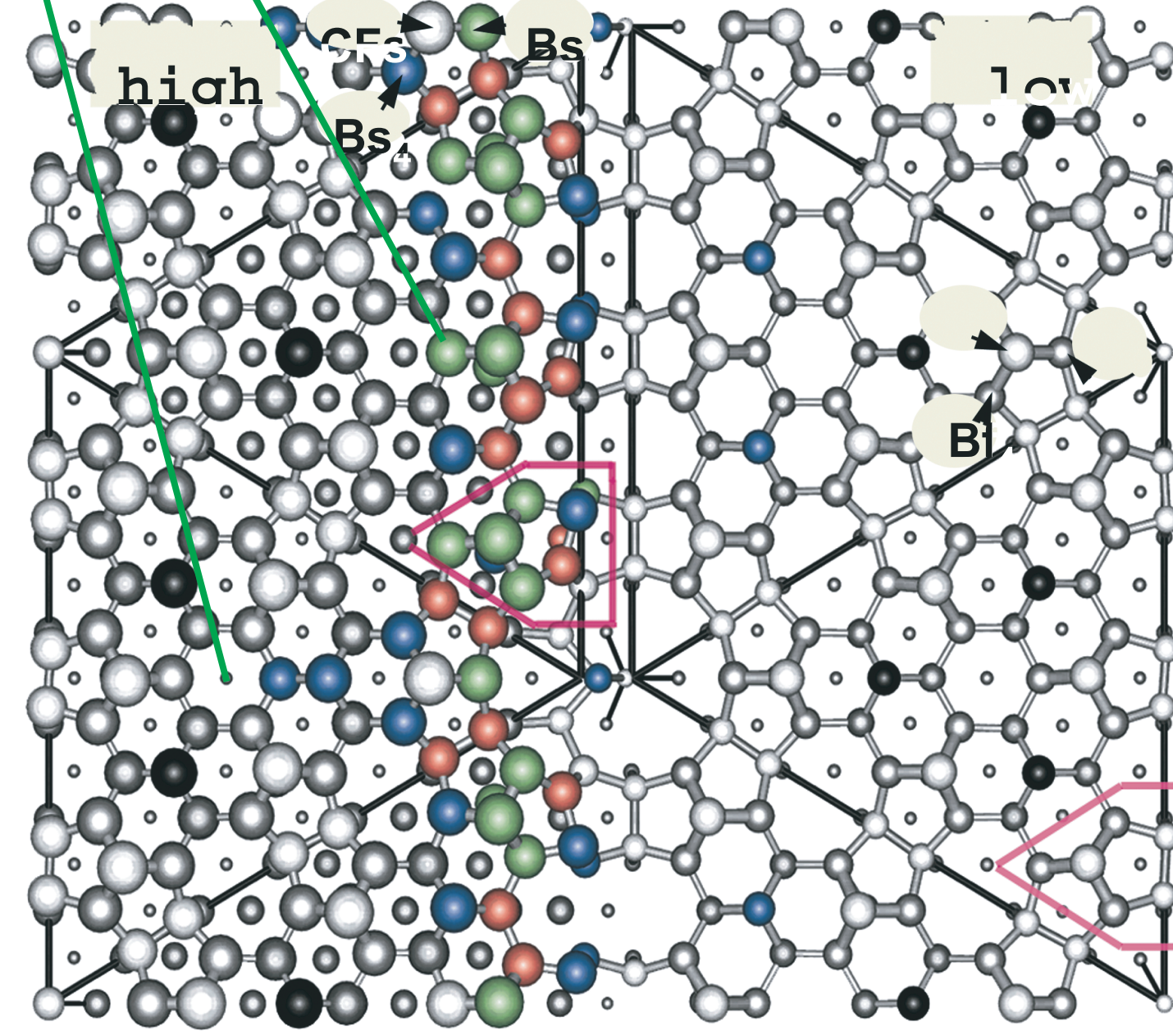
The higher density of states in FL explains the brightness of the image at -0.5eV

U00 step configuration for Si(111) - 7x7

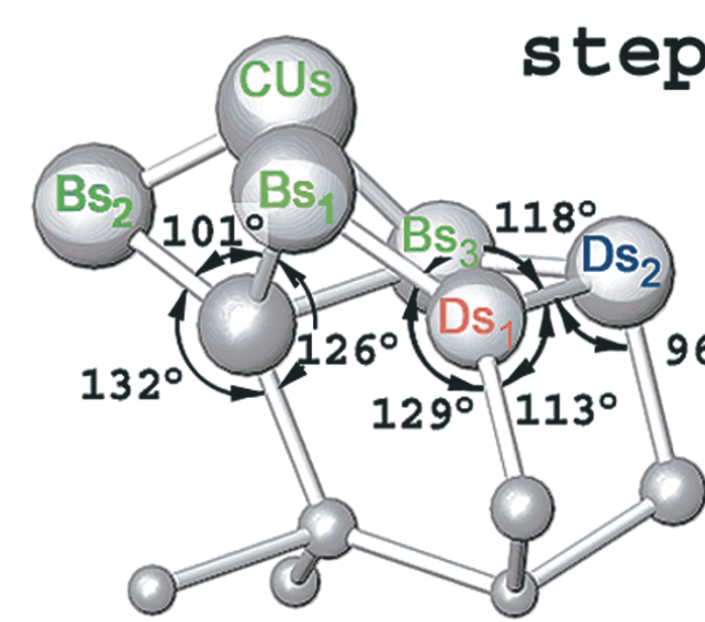
F subcell

U subcell

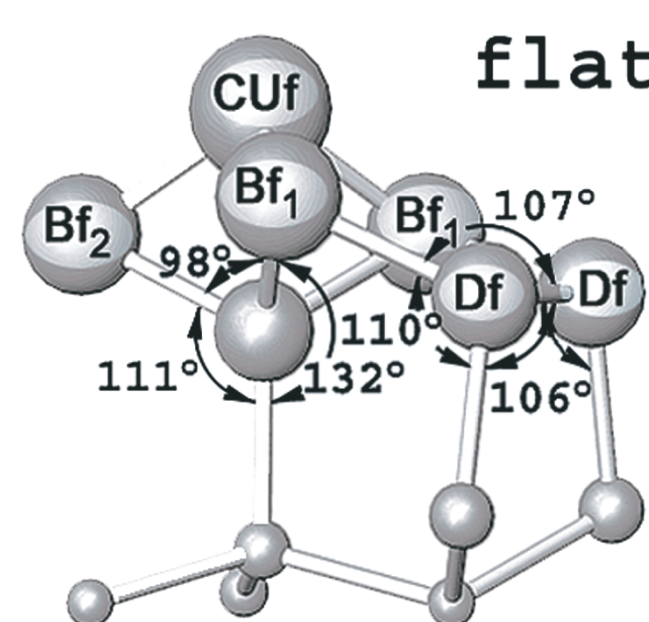
New bands are introduced because of changes in the dimer configuration. sp^2 rehybridization causes the band at +0.7eV while the $s+3p$ rehybridization causes the new occupied band -0.8 to -1eV.



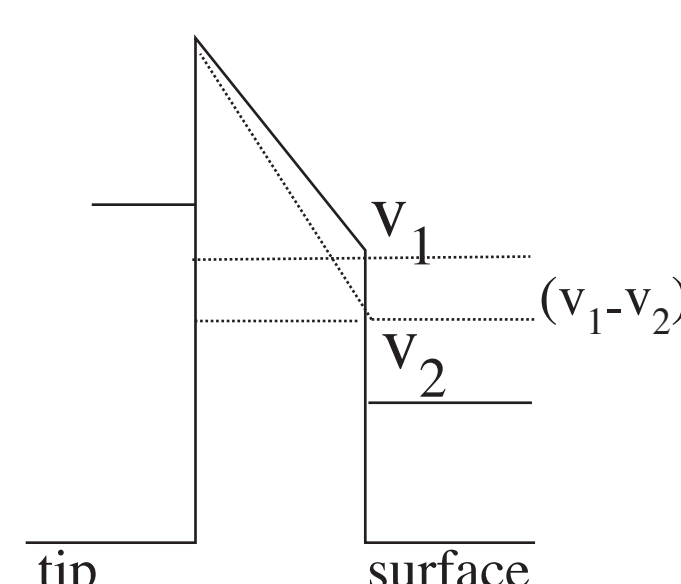
- No transition region between low and high side
- No lateral shift



- Relaxed dimer configuration at the step



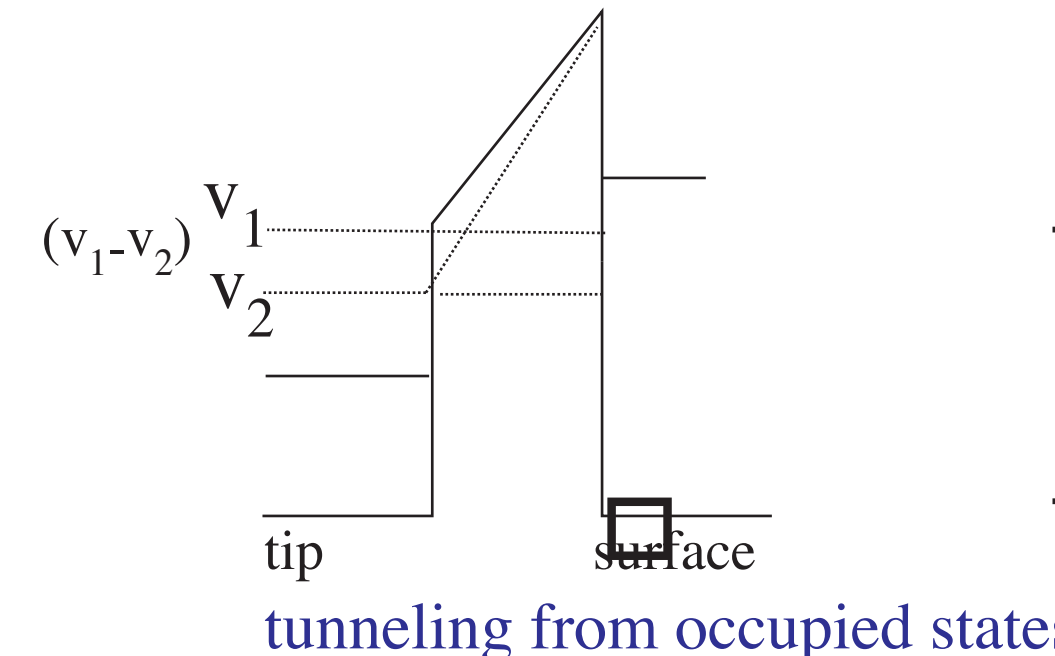
- Unrelaxed step configuration on the flat surface



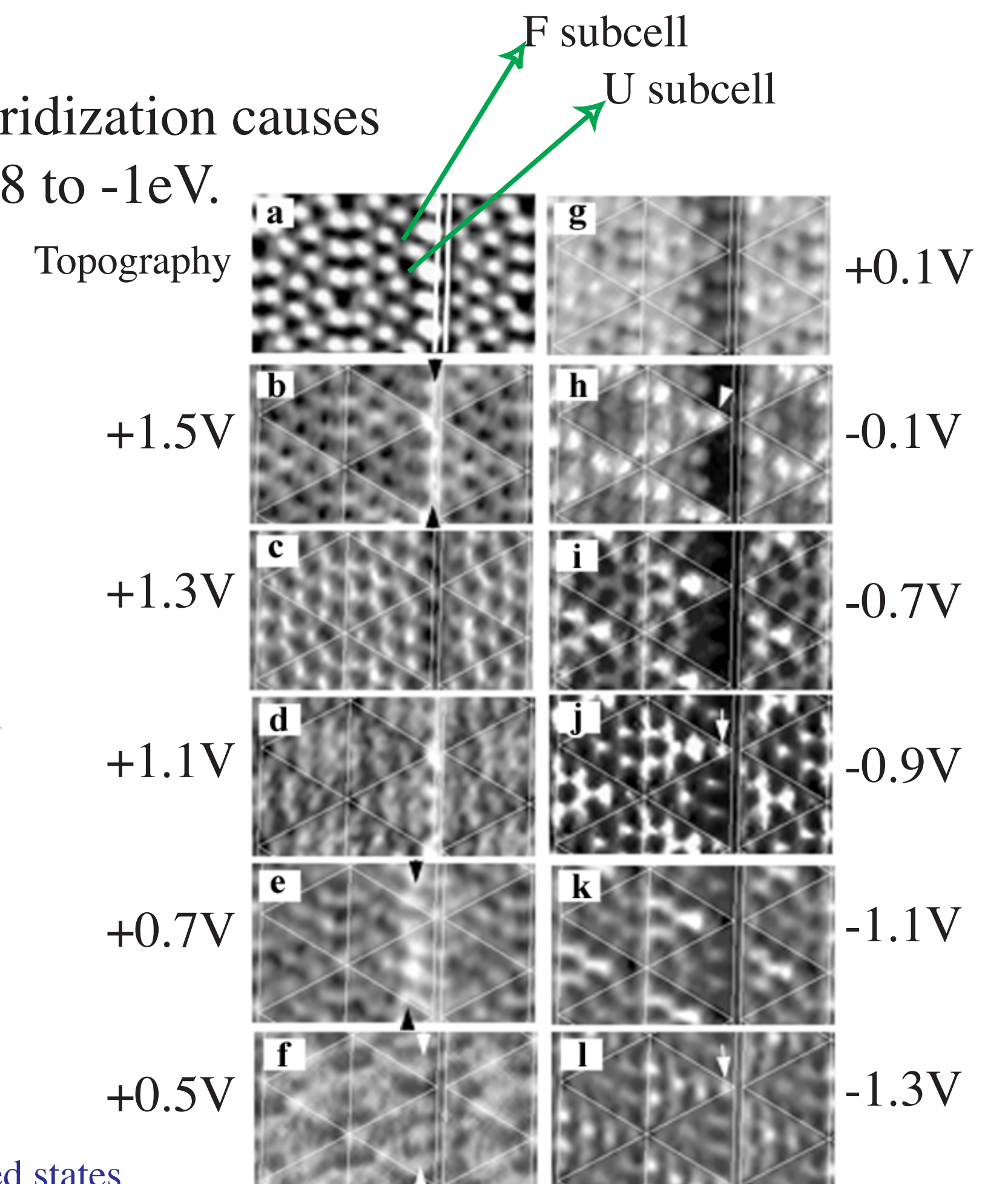
tunneling to unoccupied states

Differential Spectroscopy:

Difference between two images obtained at V_1, V_2 reveals information about the local DOS with the energy range $\Delta E = V_2 - V_1$

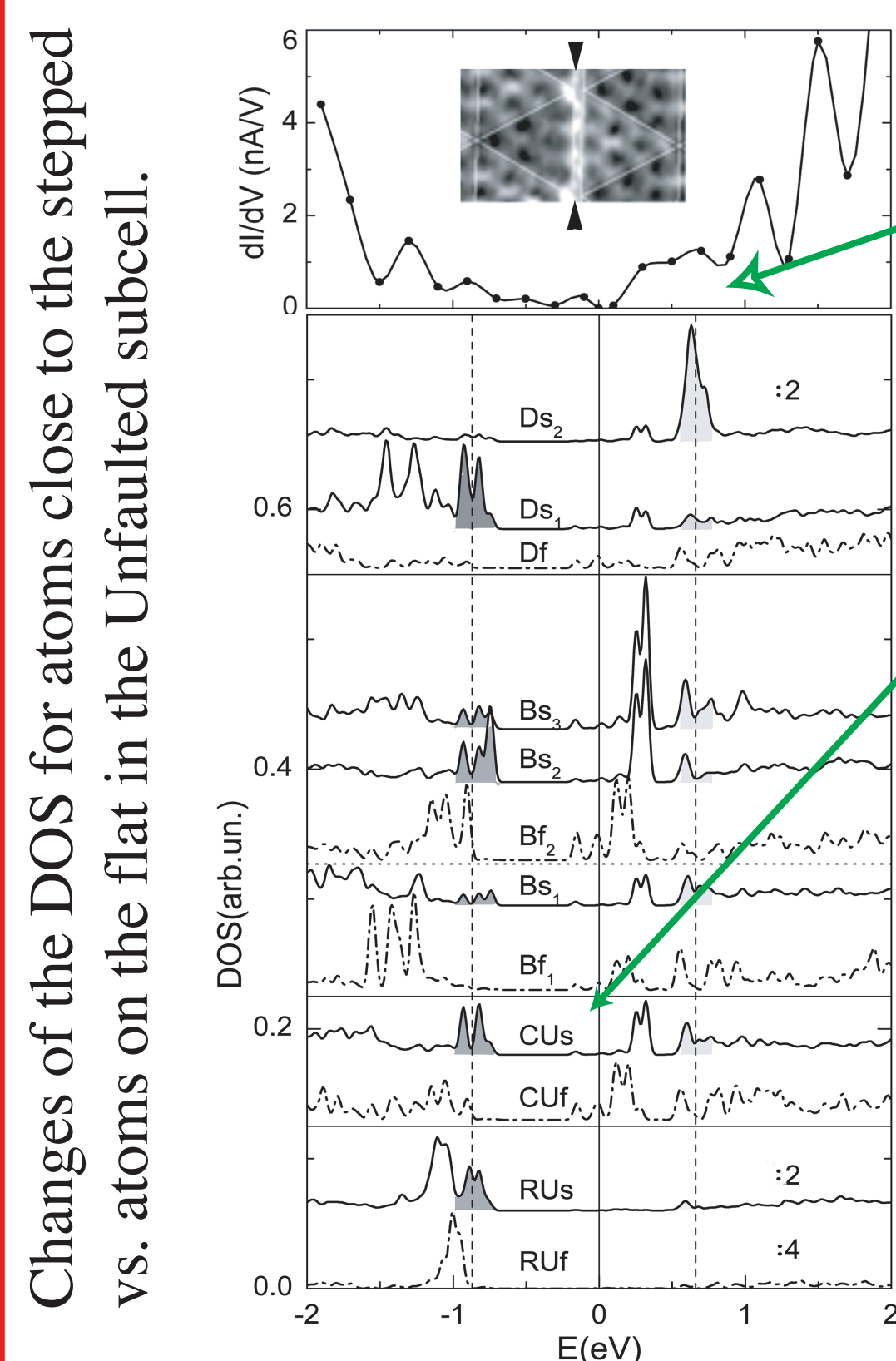


tunneling from occupied states



Differential spectroscopy for the voltages shown with $\Delta E = 0.2eV$.

Integrated spectra over the region close to the step showing the band at +0.7eV.



dimer atoms

backbone atoms

corner adatoms

restatom

Observations:

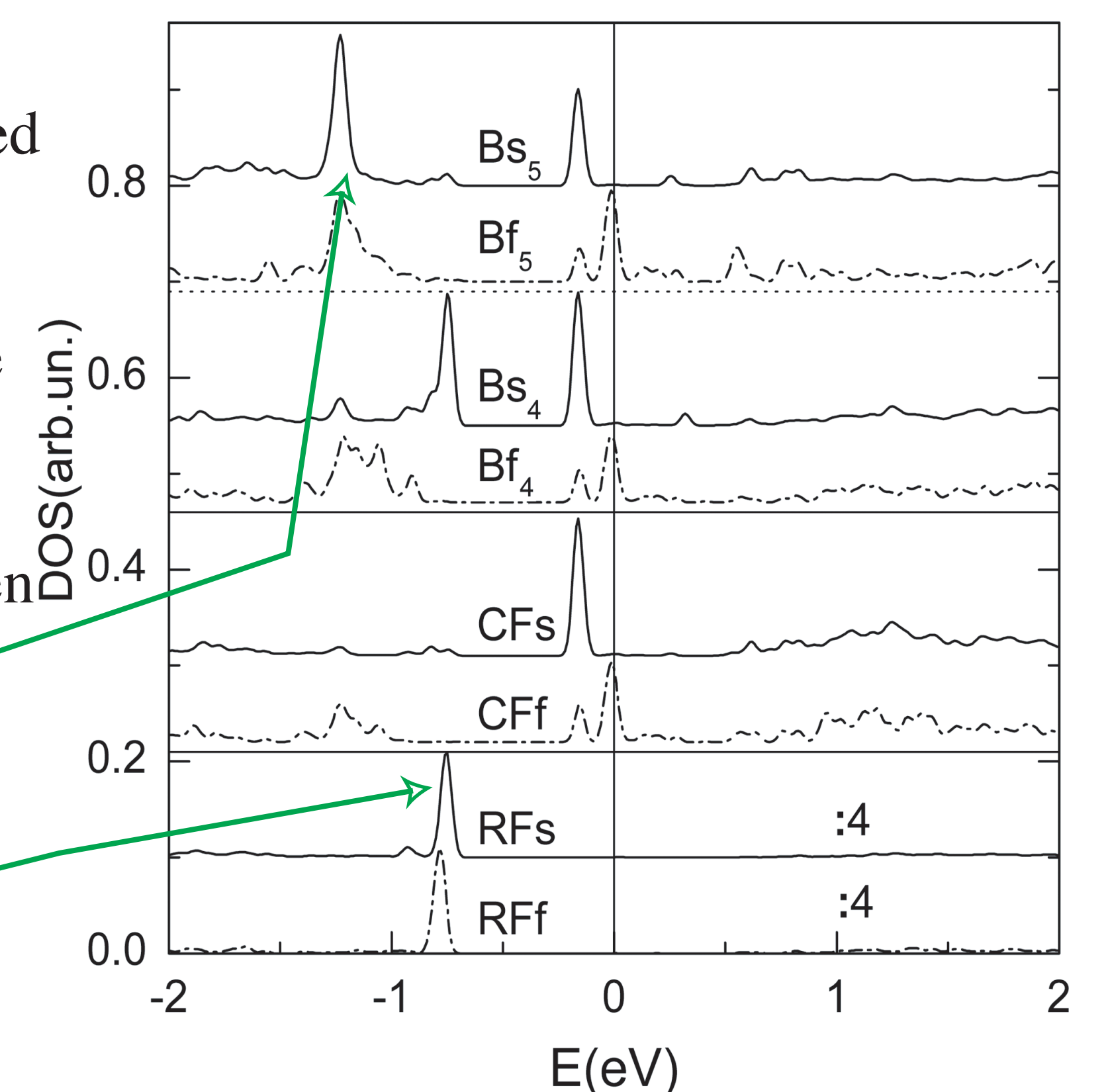
1. A band of high intensity is seen in the unoccupied states of the Unfaulted subcell at +0.7eV (b, d, e). □

2. Low intensity in the zone close to the step in the energy range -0.7eV to -0.1eV (g, h, i). □

3. Backbone states in the range -1 to -1.5 V are seen in the Faulted subcell on the high side of the step (k, l). □

4. Restatom state at -0.8eV is seen in the Faulted subcell (j). □

Calculated DOS



Faulted subcell